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NEWS 4 JUL 28 IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS 5 JUL 28 STN Viewer performance improved
NEWS 6 AUG 01 INPADOCDB and INPAFAMDB coverage enhanced
NEWS 7 AUG 13 CA/CAplus enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS 8 AUG 15 CAOLD to be discontinued on December 31, 2008
NEWS 9 AUG 15 CAplus currency for Korean patents enhanced
NEWS 10 AUG 27 CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information
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NEWS 12 SEP 25 CA/CAplus current-awareness alert options enhanced to accommodate supplemental CAS indexing of exemplified prophetic substances
NEWS 13 SEP 26 WPIDS, WPINDEX, and WPIX coverage of Chinese and and Korean patents enhanced
NEWS 14 SEP 29 IFICLS enhanced with new super search field
NEWS 15 SEP 29 EMBASE and EMBAL enhanced with new search and display fields
NEWS 16 SEP 30 CAS patent coverage enhanced to include exemplified prophetic substances identified in new Japanese-language patents
NEWS 17 OCT 07 EPFULL enhanced with full implementation of EPC2000
NEWS 18 OCT 07 Multiple databases enhanced for more flexible patent number searching
NEWS 19 OCT 22 Current-awareness alert (SDI) setup and editing enhanced
NEWS 20 OCT 22 WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT Applications
NEWS 21 OCT 24 CHEMLIST enhanced with intermediate list of pre-registered REACH substances

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                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

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DICTIONARY FILE UPDATES:   7 NOV 2008  HIGHEST RN 1071660-21-3

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http://www.cas.org/support/stngen/stndoc/properties.html

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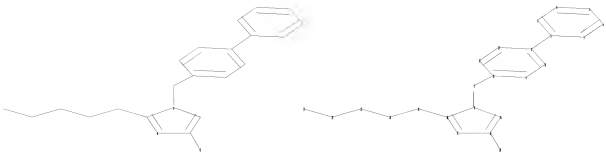

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ring nodes :
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ring bonds :
1-3 1-7 2-8 2-12 3-4 4-5 5-6 6-7 8-9 9-10 10-11 11-12 14-15 14-18
15-16 16-17 17-18
exact/norm bonds :
13-14 14-15 14-18 15-16 16-17 17-18
exact bonds :
1-2 10-13 16-24 18-19 19-20 20-21 21-22 22-23
normalized bonds :
1-3 1-7 2-8 2-12 3-4 4-5 5-6 6-7 8-9 9-10 10-11 11-12

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS

L1 STRUCTURE UPLOADED

=> d

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L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


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SAMPLE SEARCH INITIATED 23:23:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      197 TO ITERATE

100.0% PROCESSED      197 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          3098 TO     4782
PROJECTED ANSWERS:                0 TO        0

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=> l1 full
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SEARCH TIME: 00.00.01

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=> file caplus
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                                                       ENTRY    SESSION
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FILE 'CAPLUS' ENTERED AT 23:23:43 ON 09 NOV 2008
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FILE COVERS 1907 - 9 Nov 2008  VOL 149 ISS 20
FILE LAST UPDATED: 7 Nov 2008  (20081107/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.
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=> l3
L4            5 L3

=> d ibib abs hitstr 1-5

L4   ANSWER 1 OF 5  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2006:600074  CAPLUS
DOCUMENT NUMBER:          145:180201
TITLE:                    Proposal of a New Binding Orientation for Non-Peptide
                          AT1 Antagonists: Homology Modeling, Docking and
                          Three-Dimensional Quantitative Structure-Activity
                          Relationship Analysis
AUTHOR(S):                Tuccinardi, Tiziano; Calderone, Vincenzo; Rapposelli,
                          Simona; Martinelli, Adriano
CORPORATE SOURCE:         Dipartimento di Scienze Farmaceutiche, Universita di
                          Pisa, Pisa, 56126, Italy
SOURCE:                   Journal of Medicinal Chemistry (2006), 49(14),
                          4305-4316
                          CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER:                American Chemical Society
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB   A three-dimensional model of the AT1 receptor was constructed by means of
     a homol. modeling procedure, using the x-ray structure of bovine rhodopsin
     as the initial template and taking into account the available
     site-directed mutagenesis data.  The docking of losartan and its active
     metabolite EXP3174, followed by 1 ns of mol. dynamics (MD) simulation
     inserted into the phospholipid bilayer, suggested a different binding
     orientation for these antagonists from those previously proposed.
     Furthermore, the docking of several nonpeptide antagonists was used as an
     alignment tool for the development of a three-dimensional quant.
     structure-activity relationship (3D-QSAR) model, and the good results
     confirmed our binding hypothesis and the reliability of the model.
IT   114799-09-6
     RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic
     use); BIOL (Biological study); USES (Uses)
        (proposal of a new binding orientation for non-peptide AT1 antagonists
        based on homol. modeling, docking and three-dimensional quant.
        structure-activity relationship anal.)
RN   114799-09-6  CAPLUS
CN   [1,1'-Biphenyl]-2-carboxylic acid,
     4'-[[4-chloro-2-hexyl-5-(hydroxymethyl)-1H-imidazol-1-yl]methyl]-  (CA
     INDEX NAME)
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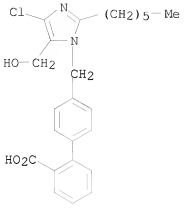


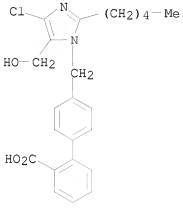
REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:619582 CAPLUS
DOCUMENT NUMBER: 135:338737
TITLE: Comparative QSAR: Angiotensin II Antagonists
AUTHOR(S): Kurup, Alka; Garg, Rajni; Carini, D. J.; Hansch, Corwin
CORPORATE SOURCE: Department of Chemistry, Pomona College, Claremont, CA, 91711, USA
SOURCE: Chemical Reviews (Washington, D. C.) (2001), 101(9), 2727-2750
CODEN: CHREAY; ISSN: 0009-2665
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

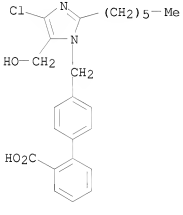
AB A QSAR study was carried out on nonpeptide angiotensin II antagonists which included a review of the literature on bioactivity and derivation of QSAR equations. The QSAR were divided into 4 groups according to the test system: rabbit, rat, guinea pig and human. Within each group, these are arranged according to potency (log I/C). Also listed is the CMR (calculated molar refractivity) which is similar to molar volume but contains a small element for polarizability, and Clog P values which give an assessment of the hydrophobic effects. The authors also used π as a measure of local hydrophobic binding sites. All the QSAR reported in the study were derived by the authors. The physicochem. parameters were autoloaded from their C-QSAR databases and the QSAR regression anal. was executed with a C-QSAR program. The authors derived 39 QSAR equations which provide an overview of the structure-activity relationship for a variety of compds. To the authors knowledge, these are the first QSAR for angiotensin antagonists. The most important conclusion reached is the lack of importance of hydrophobic interactions with the receptors. The relevance of the biphenyl moiety for hydrophobicity is discussed and a model of the pharmacophore is presented.

IT 114799-08-5 114799-09-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(comparative QSAR of nonpeptide angiotensin II antagonists)
RN 114799-08-5 CAPLUS

CN [1,1'-Biphenyl]-2-carboxylic acid,
4'-[[4-chloro-5-(hydroxymethyl)-2-pentyl-1H-imidazol-1-yl]methyl]- (CA INDEX NAME)



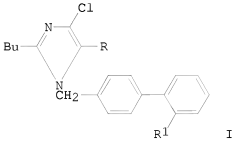
RN 114799-09-6 CAPLUS
CN [1,1'-Biphenyl]-2-carboxylic acid,
4'-[[4-chloro-2-hexyl-5-(hydroxymethyl)-1H-imidazol-1-yl]methyl]- (CA INDEX NAME)



REFERENCE COUNT: 73 THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

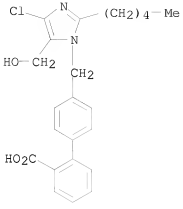
L4 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:492147 CAPLUS
DOCUMENT NUMBER: 115:92147
ORIGINAL REFERENCE NO.: 115:15855a,15858a
TITLE: Nonpeptide angiotensin II receptor antagonists: the discovery of a series of N-(biphenylylmethyl)imidazoles as potent, orally active antihypertensives
AUTHOR(S): Carini, David J.; Duncia, John V.; Aldrich, Paul E.; Chiu, Andrew T.; Johnson, Alexander L.; Pierce, Michael E.; Price, William A.; Santella, Joseph B.,

III; Wells, Gregory J.; et al.
CORPORATE SOURCE: Pharm. Div., E. I. Du Pont de Nemours and Co., Inc., Wilmington, DE, 19880-0402, USA
SOURCE: Journal of Medicinal Chemistry (1991), 34(8), 2525-47
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

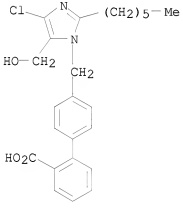


I

AB Nonpeptide angiotensin II receptor antagonists I (R = CH2OH, CH2OMe, CHO; R1 = tetrazolyl, (un)substituted triazolyl, CO2H, CONHR2, R2 = OH, OMe, OCH2Ph, SO2Ph, NHSO2CF3, COCF3, SO2CF3) were prepared and produced a potent antihypertensive effect upon oral administration. The acidic group at the 2'-position of the biphenyl is essential. Only ortho-substituted acids possess both high affinity for the AII receptor and good oral antihypertensive potency. The carboxylic acid group has been replaced with a variety of acidic isosteres, and the tetrazole ring was the most effective.
IT 114799-08-5P 114799-09-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antihypertensive activity of)
RN 114799-08-5 CAPLUS
CN [1,1'-Biphenyl]-2-carboxylic acid, 4'-[[4-chloro-5-(hydroxymethyl)-2-pentyl-1H-imidazol-1-yl]methyl]- (CA INDEX NAME)



RN 114799-09-6 CAPLUS
CN [1,1'-Biphenyl]-2-carboxylic acid, 4'-[[4-chloro-2-hexyl-5-(hydroxymethyl)-1H-imidazol-1-yl]methyl]- (CA INDEX NAME)



L4 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:118817 CAPLUS
DOCUMENT NUMBER: 112:118817
ORIGINAL REFERENCE NO.: 112:20131a,20134a
TITLE: Preparation of (biphenylylmethyl)imidazoles and analogs as antihypertensive agents
INVENTOR(S): Carini, David John; Wong, Pancras Chor Bun; Duncia, John Jonas Vytautas
PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA
SOURCE: Eur. Pat. Appl., 271 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

EP 324377	A2	19890719	EP 1989-100144	19890105
EP 324377	A3	19910206		
EP 324377	B1	19970416		
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US 5138069	A	19920811	US 1988-279194	19881206
CA 1338238	C	19960409	CA 1988-586904	19881222
WO 8906233	A1	19890713	WO 1989-US52	19890105
W: JP				
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EP 733366	A2	19960925	EP 1996-107930	19890105
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EP 733366	B1	19980401		
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ES 2100150	T3	19970616	ES 1989-100144	19890105
AT 164520	T	19980415	AT 1996-107930	19890105
ES 2117463	T3	19980801	ES 1996-107930	19890105
DK 8900051	A	19890708	DK 1989-51	19890106
DK 174948	B1	20040315		
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FI 99012	B	19970613		
FI 99012	C	19970925		
NO 8900075	A	19890710	NO 1989-75	19890106
NO 177265	B	19950508		
NO 177265	C	19950816		
AU 8927771	A	19890713	AU 1989-27771	19890106
AU 617736	B2	19911205		
ZA 8900127	A	19900926	ZA 1989-127	19890106
SU 1814646	A3	19930507	SU 1989-4613475	19890106
HU 64038	A2	19931129	HU 1989-50	19890106
HU 218201	B	20000628		
US 5128355	A	19920707	US 1989-435869	19891113
US 5153197	A	19921006	US 1989-436165	19891113
US 5155118	A	19921013	US 1989-436281	19891113
RU 2017733	C1	19940815	RU 1992-5010637	19920127
US 5210079	A	19930511	US 1992-832638	19920207
US 5354867	A	19941011	US 1993-47883	19930415

PRIORITY APPLN. INFO.:

US 1988-142580	A	19880107
US 1988-279194	A	19881206
US 1986-884920	B2	19860711
US 1987-50341	B2	19870522
EP 1989-100144	A3	19890105
WO 1989-US52	W	19890105
US 1989-373755	B2	19890630
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OTHER SOURCE(S): MARPAT 112:118817

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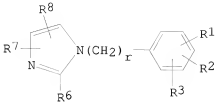

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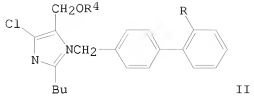


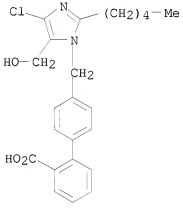
II

AB The title compds. [I; R1 = acyl, tetrazolyl, aminoacyl, acylamino, biphenylyl, etc.; R2 = H, halo, NO2, cyano, C1-4 alkyl, etc.; R3 = H, halo, C1-4 alkyl, alkoxy; R6 = C2-10 alkyl, C3-10 alkenyl, alkynyl, C3-8 cycloalkyl, (un)substituted Ph, PhCH2, etc.; R7 = H, halo, NO2, cyano, pentafluorophenyl, etc.; R8 = H, cyano, C1-10 (fluoro)alkyl, etc.; r = 0-2] were prepared Thus, 2-butyl-4-chloro-5-hydroxymethylimidazole was stirred 0.5 h with NaOMe in MeOH and the product stirred overnight with 4'-bromomethyl-2-cyanobiphenyl (preparation given) in DMF to give title compound II (R = cyano, R4 = H) which was converted in 2 steps to II (R = cyano, R4 = Me). The latter was stirred 2 days at 100° and 11 days at 120° with NaN3 in DMF containing NH4Cl to give II (R = 1H-tetrazol-5-yl, R4 = Me) the Na salt of which had IC50 of 0.020 μM for inhibition of angiotensin II receptor binding and showed significant decreases in blood pressure in rats at ≤10 and ≤100 mg/kg i.v. and orally, resp.

IT 114799-08-5P 114799-09-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antihypertensive agent)

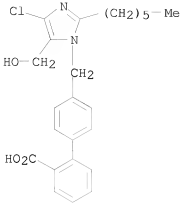
RN 114799-08-5 CAPLUS

CN [1,1'-Biphenyl]-2-carboxylic acid, 4'-[[4-chloro-5-(hydroxymethyl)-2-pentyl-1H-imidazol-1-yl]methyl]- (CA INDEX NAME)



RN 114799-09-6 CAPLUS

CN [1,1'-Biphenyl]-2-carboxylic acid, 4'-[[4-chloro-2-hexyl-5-(hydroxymethyl)-1H-imidazol-1-yl]methyl]- (CA INDEX NAME)



L4 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:529008 CAPLUS
DOCUMENT NUMBER: 109:129008
ORIGINAL REFERENCE NO.: 109:21501a,21504a
TITLE: Preparation of angiotensin II receptor-blocking (phenylalkyl)imidazoles
INVENTOR(S): Carini, David John; Duncia, John Jonas Vytautas
PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA
SOURCE: Eur. Pat. Appl., 314 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 253310	A2	19880120	EP 1987-109919	19870709
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CA 1334092	C	19950124	CA 1987-540399	19870623
NO 8702863	A	19880112	NO 1987-2863	19870709
NO 176049	B	19941017		
NO 176049	C	19950125		
ES 2063734	T3	19950116	ES 1987-109919	19870709
DK 8703596	A	19880112	DK 1987-3596	19870710
DK 174700	B1	20030922		
FI 8703071	A	19880112	FI 1987-3071	19870710
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AU 599396	B2	19900719		
JP 63023868	A	19880201	JP 1987-171328	19870710
JP 05029351	B	19930430		
HU 45976	A2	19880928	HU 1987-3174	19870710
ZA 8705052	A	19890329	ZA 1987-5052	19870710
SU 1694062	A3	19911123	SU 1987-4203085	19870710
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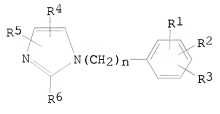
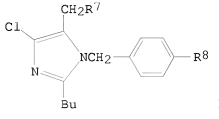
OTHER SOURCE(S): MARPAT 109:129008

GI



I



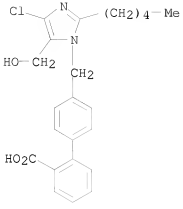
II

AB The title compound [I; R1 = tetrazol-5-yl, 1,2,3-triazol-4-yl, (HO)2S(O)O, (HO)2P(O)O, HPO3, substituted NH2, alkyl, PhCH2, (un)substituted PhCH2CH2, PhCH:CH, (un)modified CO2H, SO3H, etc.; R2 = H, C1-4 alkyl, C1-4 alkoxy, C1-4 acyloxy, MeSO2NH, CF3SO2NH, aryl, furyl, tetrazol-5-yl, Br, Cl, F, iodo, NO2, (un)modified CO2H; R3 = H, C1-4 alkyl, C1-4 alkoxy, Br, Cl, F, iodo; R4 = H, CF3, cyano, Br, Cl, F, iodo; R5 = H, cyano, (un)substituted alkyl, alkenyl; n = 0-2] and their pharmaceutically acceptable salts were prepared as angiotensin II receptor-blocking agents, useful as antihypertensives. 2-Butyl-5-chloro-1H-imidazole-4-methanol was treated with NaOMe in MeOH, and N-alkylated with 4-BrCH2C6H4CN to give benzylimidazolemethanol II (R7 = OH, R8 = cyano). This was chlorinated with SOCl2 and treated with NaCN to give II (R7 = R8 = cyano). The latter was refluxed 6 h in 1:1 12N HCl/HOAc to give II (R7 = R8 = CO2H) (III). III inhibited angiotensin II binding in rat adrenal cortical microsomes with an IC50 of 1.80 μM and was active in reducing blood pressure in rats at 10 mg/kg i.v.

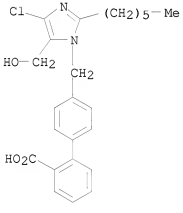
IT 114799-08-5P 114799-09-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antihypertensive)

RN 114799-08-5 CAPLUS

CN [1,1'-Biphenyl]-2-carboxylic acid, 4'-[[4-chloro-5-(hydroxymethyl)-2-pentyl-1H-imidazol-1-yl]methyl]- (CA INDEX NAME)



RN 114799-09-6 CAPLUS
CN [1,1'-Biphenyl]-2-carboxylic acid,
4'-[[4-chloro-2-hexyl-5-(hydroxymethyl)-1H-imidazol-1-yl]methyl]- (CA
INDEX NAME)



=> log h
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	27.73	206.30
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.00	-4.00

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 23:24:34 ON 09 NOV 2008